Quantum Monte Carlo calculations of symmetric nuclear matter

Stefano Gandolfi,[1] Francesco Pederiva,[1,2] Stefano Fantoni,[3,2] and Kevin E. Schmidt[4]

[1] *Dipartimento di Fisica and INFN, University of Trento, via Sommarive 14, I-38050 Povo, Trento Italy*
[2] *CNR–DEMOCRITOS National Supercomputing Center, Trieste, Italy*
[3] *S.I.S.S.A., International School of Advanced Studies and INFN via Beirut 2/4, 34014 Trieste, Italy*
[4] *Department of Physics, Arizona State University, Tempe, AZ, USA*

We present an accurate numerical study of the equation of state of nuclear matter based on realistic nucleon–nucleon interactions by means of Auxiliary Field Diffusion Monte Carlo (AFDMC) calculations. The AFDMC method samples the spin and isospin degrees of freedom allowing for quantum simulations of large nucleonic systems and represents an important step forward towards a quantitative understanding of problems in nuclear structure and astrophysics.

The equation of state (EOS) of nuclear matter represents a challenge in both nuclear structure physics and astrophysics. The knowledge of the properties of nuclear matter, and in particular of asymmetric nuclear matter, is needed to predict the structure, the dynamics and the evolution of stars, in particular during their last stages, when they become ultra–dense neutron stars. Depending on the EOS, the density of nuclear matter in the inner shells can reach up to 9 times the core density of stable nuclei, $\rho_0 = 0.16$ fm^{-3}[1].

One important step towards the understanding of these astrophysical problems is the study of the symmetric nuclear matter, related to the various model NN interactions available. While considerable advances have been made[2, 3], it is still impossible to firmly ascertain the degree of accuracy of the approximations one has to introduce in the many-body theories, and substantial discrepancies still exist among the different theoretical estimates of the EOS, the response functions and Green's Functions of nuclear matter.

Experimental data on symmetric nuclear matter are limited to the volume and the symmetry energy of the Weizsacker mass formula, and to the nuclear matter compressibility. Instead, an indirect test for the theoretical predictions of the EOS of asymmetric nuclear matter is provided by the mass–radius relation of a neutron star[3, 4, 5], obtained by solving the Tolman-Oppenheimer-Volkov equation.

At present the theoretical uncertainties on the equation of state, coming from the approximations one has to introduce in the many-body methods, and the lack of knowledge of the nuclear interaction, do not allow for definite conclusions when comparing with astronomical observations. However, the recent success in predicting the properties of light nuclei gives us some confidence that the non–relativistic description of nuclear matter based on effective potentials fitted to reproduce NN data and the binding energy of light nuclei can be reliable enough. The main feature of such nucleon–nucleon interactions, besides the short range repulsion, is the explicit dependence on the relative quantum state of the nucleons which can be described using spin and isospin, angular momentum, spin–orbit, and tensor operators[6].

Properties of light nuclei (A$\leq$6) can be efficiently computed with high accuracy using modern few–body techniques[7, 8, 9] or with the ab initio no-core nuclear shell model (with A$\leq$12[10]). Quantum Monte Carlo techniques based on recasting the Schroedinger equation into a diffusion equation (Diffusion Monte Carlo or Green's Function Monte Carlo), allowed for performing calculations up to A$\leq$12[11, 12]. However, the computational resources needed for such simulations are very large, because of the summation over all the possible states necessary to evaluate the terms of the Hamiltonian with a quadratic dependence on spin and isospin. The number of such terms, and the CPU time needed to calculate them, grows exponentially with the number of nucleons; ^{12}C[11] or 14 neutrons[13] is the limit for the currently available computational resources.

Since the spatial degrees of freedom are already sampled, one would like to replace the sum over the spin–isospin states with an efficient sampling method. The simulation of symmetric nuclear matter requires a minimum of 28 nucleons in a box replicated in space (7 nucleons for each spin–isospin state) to obtain a wave function with closed shells of momenta, and this is out of the reach of the standard Quantum Monte Carlo methods.

In this paper we show that the spin–isospin is efficiently sampled by using the Auxiliary Field Diffusion Monte Carlo method[14], which is based on the use of auxiliary variables to linearize the quadratic spin–isospin operators of the nuclear matter Hamiltonian, making them treatable in a diffusion Monte Carlo scheme. Up to now it has been applied to simulate pure neutron matter (up to 114 neutrons)[15, 16], and neutron drops[17, 18] interacting with realistic two– plus three–body interactions.

Here we extend calculations to include isospin degrees of freedom and to deal with the strong tensor–isospin force, responsible of the nuclear binding. The method can readily handle an asymmetry in the number of neutron and protons or the deformation of heavy nuclei.

In this letter we show that simulations of symmetrical nuclear matter interacting via a semiphenomenological two–body interaction including spin–isospin depen-

dent and tensor components have led to an EOS which shows significant differences with respect to that obtained within Fermi Hypernetted Chain and Brueckner Hartree Fock methods[19], particularly at high densities. Even more important is the finding that Quantum Monte Carlo simulations do not lead to any lowering of the FHNC or BHF energies at $\rho \sim \rho_0$. This fact points toward an inadequacy of commonly used three-nucleon interaction models in the whole range of density.

Auxiliary Field Diffusion Monte Carlo (AFDMC)[14] is an extension of the standard Diffusion Monte Carlo method in which the ground state of an Hamiltonian H is obtained by solving the imaginary time dependent Schroedinger equation

$$-\frac{\partial}{\partial t}\Psi(X,t) = H\Psi(X,t). \qquad (1)$$

The solution is obtained by evolving a population of configurations of the system ("walkers") $X = \{R, \sigma, \tau\}$, where $R = \{\vec{r}_1, \ldots, \vec{r}_N, \}$, $\sigma = \{\vec{\sigma}_1, \ldots, \vec{\sigma}_N\}$, and $\tau = \{\vec{\tau}_1, \ldots, \vec{\tau}_N\}$, with $F(X,t) = \Psi_T(X)\Psi(X,t)$, according to

$$F(X,t) = \int dX' \frac{\Psi_T(X)}{\Psi_T(X')} G_0(X,X',t)F(X',0) \qquad (2)$$

The function Ψ_T is a "trial" wave function, usually determined by means of variational calculations, and G_0 is an approximation to the Green's function of the imaginary time Schroedinger equation:

$$G_0(X,X',t) = (4\pi Dt)^{-3A/2} e^{-(R-R')^2/4Dt} e^{-t(V(X)-E_0)}, \qquad (3)$$

where $D = \hbar^2/2m$, E_0 is an estimate of the ground state energy of the system, and $V(X)$ is the nucleon–nucleon interaction. For a long enough imaginary time the distribution of the walkers converges to the product $\Psi_T(X)\Psi_0(X)$ where Ψ_0 is the wave function of the ground state of H. This fact allows the computation of matrix elements $\langle\Psi_T|\hat{O}|\Psi_0\rangle$ of observables $\hat{O}$ of interest in a Monte Carlo way. When $\hat{O} \equiv \hat{H}$ the value obtained is the exact ground state energy of the system. The presence of an interaction $V(X)$ including operators like $(3\vec{\sigma}_i \cdot \hat{r}_{ij}\vec{\sigma}_j \cdot \hat{r}_{ij} - \vec{\sigma}_i \cdot \vec{\sigma}_j)$ and $\vec{\tau}_i \cdot \vec{\tau}_j$ is the origin of the computational cost in the standard approaches. The spin-isospin dependent part of $V(X)$ (V_{sid}) can be written as a sum of a matrix $A_{i\alpha,j\beta}$ multiplied by spin-isospin operators as follow:

$$V_{sid} = \frac{1}{2}\sum_{i\alpha,j\beta} \sigma_{i\alpha} A_{i\alpha,j\beta}\sigma_{j\beta}\vec{\tau}_i \cdot \vec{\tau}_j = \frac{1}{2}\sum_{\alpha=1}^{3}\sum_{n=1}^{3A} \hat{S}_{n\alpha}^2 \lambda_n, \qquad (4)$$

where λ_n are the eigenvalues obtained by diagonalizing the matrix A, and $\hat{S}_{n\alpha}$ are operators written in terms of eigenvectors of A as follow:

$$\hat{S}_{n\alpha} = \sum_i \tau_{i\alpha}\vec{\sigma}_i \cdot \vec{\psi}_n(i) \qquad (5)$$

AFDMC uses the Hubbard–Stratonovich method to transform the operators $\hat{S}$ which are quadratic in the spin and isospin into linear operators:

$$e^{-(1/2)t\lambda\hat{S}^2} = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} dy e^{-y^2/2} e^{y\sqrt{-\lambda t}\hat{S}} \qquad (6)$$

Then $\hat{S}$ are operators which are linear combinations of the spin and isospin operators for each nucleon, and λ depend on the interaction. The transformed Green's Function is applied to the spin-isospin part of the wave function, and its effect consists of a rotation of the spin and isospin degrees of freedom (written as four-component spinors in the proton-neutron up-down basis) by a quantity that depends on the auxiliary variable y along with multiplication of the state by an overall factor. The sum over spin and isospin is replaced by sampling a set of rotations of the variables. This procedure reduces the dependence of the computational time on the number of nucleons necessary for performing a simulation step from exponential to cubic. It is therefore possible to perform on a regular workstation or on a modest PC cluster calculations that would require Tflop supercomputers with the standard methods. This method, like other diffusion Monte Carlo methods, suffers from the so–called "sign problem" when it is applied to fermions, and when complex wave functions need to be used. In our calculations we apply the fixed-phase approximation to overcome this problem[20]. While this method has already been successfully applied to pure neutron matter[16], it has not been previously used for mixed proton and neutron systems. It should be noted that it does not guarantee an upperbound to the mixed energy used here. As a test for the correctness and the efficiency of our approach we reproduced within 0.3 MeV total energy the existing results for the binding energy of ^{4}He with potentials of the v_6 class[21]. We have also been able to compute binding energies for ^{16}O with this method.

A crucial point in dealing with nuclear matter is the choice of the interaction among nucleons. As already mentioned, several modern two–body potentials are available nowadays, all fitting the NN data with $\chi^2 \sim 1$. We use the potentials of the Argonne class with n operators (AVn)[22]. While the full version contains $n = 18$ operators, most of the physics is reasonably well described by the first 6 operators made up of 4 central spin–isospin dependent components and two tensor ones, which include the long range one–pion–exchange force. The most important missing terms are the spin–orbit components. In nuclei and neutron drops the spin–orbit contribution to the energy amounts to a few tenths of MeV/nucleon. A correction of the order 1MeV/nucleon can be attributed at low densities to the remaining terms included in AV18. Specifically, we have used the interaction Argonne v_8'[21] truncated by dropping the spin–orbit terms, and including only the first six operators, which we denote as "our AV6'" .

TABLE I: AFDMC energies per particle in MeV of 28, 76 and 108 nucleons in a periodic box at various densities.

ρ/ρ_0	E/A(28)	E/A(76)	E/A(108)
0.5	-7.64(3)	-7.7(1)	-7.45(2)
3.0	-10.6(1)	-10.7(6)	-10.8(1)

It is well known that two–body NN interaction underbind light nuclei, and one needs to add a specific effective three–body potential to reproduce their low energy properties. Semi–phenomenological three–nucleon interactions following the lowest order three–nucleon diagrams with one and two intermediate Delta resonance states provide a very satisfactory description of the ground state energy and the low level spectra of light nuclei up to ^{12}C[11]. We have disregarded such three–body forces in our simulations. In nuclear matter they are essential to reproduce the experimental saturation density, and, in general, they contribute about 10% of the total binding energy. A full comparison with the available experimental data goes beyond the scopes of the present paper. Here we are interested in showing the efficiency of the AFDMC methods in dealing with nuclear matter models which include realistic tensor interactions like in our AV6' potential. Nuclear matter calculations with Argonne v_8' and Urbana three-nucleon interaction are in progress.

The results of the calculations with A=28 include box corrections that have computed by adding to the two body sums contribution of nucleons in the first shell of periodic cells. Such procedure is effective. In order to assess the magnitude of finite size effects we performed calculations with 76 and 108 nucleons at densities $\rho = 0.08$ fm^{-3} and $\rho = 0.48$ fm^{-3}. Results are shown in table I. As it can be seen the results coincide with the ones obtained with 28 nucleons within 3 percent.

In the case of 28 nucleons for each density we generated and then propagated a set of 1000 walkers for different time-steps ranging from $\Delta t = 5 \times 10^{-6}$MeV^{-1} to $\Delta t = 2.5 \times 10^{-5}$MeV^{-1}. Each propagation at each time-step were performed up to at least a total imaginary time of $t = 2$MeV^{-1}. The AFDMC energy is determined by extrapolating to $\Delta t \to 0$. In order to lower statistical errors, in some case longer total propagation time was needed, up to a maximum of $t = 6$MeV^{-1} in particular at higher densities. Using a parallel supercomputer (typically 16 CPU are employed) a propagation of 20000 steps requires about 80 processor hours. Then for a fixed density we estimated that a maximum of 5000 CPU hours are needed. In the case of 76 and 108 nucleons we performed calculations only at a one time-step $\Delta t = 10^{-5}$MeV^{-1} and we propagated until a total imaginary time of $t = 1$MeV^{-1}.

We computed the EOS of symmetric nuclear matter in the range of densities $0.5 \leq (\rho/\rho_0) \leq 3$, and compared it with previous available results obtained with the same potential using Fermi Hypernetted Chain in the Single Operator Chain approximation (FHNC/SOC) and the Brueckner-Hartree-Fock (BHF) in the two–hole line approximation[19]. AFDMC calculations were performed with 28 nucleons, filling the shell of plane waves with momentum of modulus 1 and providing a wave function yielding an isotropic density.

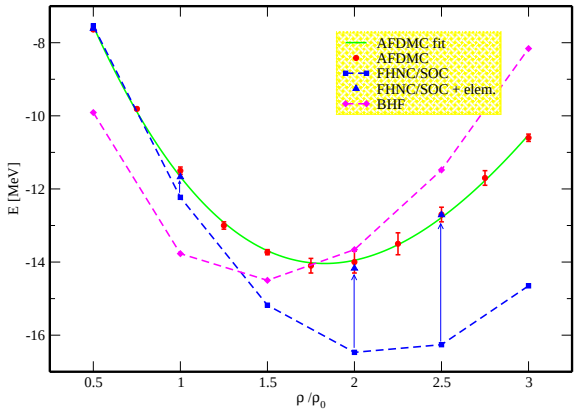

FIG. 1: (color online). Equation of state of symmetric nuclear matter calculated with different methods. Red circles represent AFDMC results with statistical error bars and the green line is the fitted functional form described in the text. Dashed lines correspond to calculations performed with other methods[19] (blue line with squares: FHNC/SOC; magenta with diamonds: BHF). Blue triangles represent the FHNC/SOC energies corrected by including the low order of elementary diagrams as described in the text. Blue arrows show the corresponding energy shift, which increases at higher densities.

The results are summarized in Fig. 1 and reported in Table II. The comparison of the various EOS suggests the following comments: FHNC/SOC leads to an overbinding at high density. A similar indication was found by Moroni et al.[23] after a DMC calculation of the EOS of normal liquid ^{3}He at zero temperature, with a guiding function including triplet and backflow correlations. The comparison with the equivalent FHNC/SOC calculations of refs[24, 25] have shown similar discrepancies. There are two main intrinsic approximations in variational FHNC/SOC calculations, which violate the variational principle. The first one consists in neglecting a whole class of cluster diagrams, the so called *elementary diagrams*, which cannot be summed up by means of FHNC integral equations. We have calculated the lowest order diagram of this class, namely the one having only one correlation bond and four exchange bonds. The results obtained show a substantial effect from this diagram and bring the FHNC/SOC estimates very close to AFDMC results, as shown in Fig. 1. The second approximation is related to the non-commutativity of the correlation operators entering the variational wave function.

TABLE II: AFDMC energies per particle in MeV of 28 nucleons in a periodic box at various densities.

ρ/ρ_0	0.5	0.75	1.0	1.25	1.5	1.75
E/A	-7.64(3)	-9.81(4)	-11.5(1)	-13.0(1)	-13.73(7)	-14.1(2)
ρ/ρ_0	2.0	2.25	2.5	2.75	3.0	
E/A	-14.0(3)	-13.5(3)	-12.7(2)	-11.7(2)	-10.6(1)	

The only class of cluster diagrams contributing to such non-commuting terms, which can be realistically calculated, is that characterized by single operator chains. It is believed that such an approximation is reliable in nuclear matter, but there is no clear proof of this.

BHF calculations of ref.[19] predict an EOS with a shallower binding than the AFDMC one. It has been shown for symmetric nuclear matter, using the AV18 and AV14 potentials, that contributions from three hole–line diagrams add a repulsive contribution up to $\sim$ 3MeV at densities below ρ_0[26], and decrease the energy at high densities[27]. Such corrections, if computed with our AV6' potential, would probably preserve the same general behavior, and bring the BHF EOS closer to the AFDMC one. Therefore, our calculations show that the two hole–line approximation used in Ref. [19] is too poor, particularly at high density.

The AFDMC equation of state was fitted with the following functional form:

$$\frac{E}{A} = \frac{E_0}{A} + \alpha(x-\bar{x})^2 + \beta(x-\bar{x})^3, \qquad (7)$$

where $x = \rho/\rho_0$ and the various coefficients are given by E_0/A = -14.04(4) MeV, α = 3.09(6) MeV, β = -0.44(8) MeV, and $\bar{x}$ = 1.83(1). The resulting compressibility $K = 9\bar{x}^2 \left(\partial^2 \left(E/A\right)/\partial x^2\right)_{\bar{x}}$ at saturation density $\bar{x}$ is $\sim$ 190 MeV. The fit of the EOS allows for computing the pressure vs. density for symmetric nuclear matter.

The availability of an efficient and relatively fast projection algorithm for the computation of energies and other observables of dense hadronic matter enables the possibility of a more quantitative understanding of the properties of neutron stars and supernovae, as well as that of medium–heavy nuclei. Computations on such systems are at present out of reach of the standard GFMC methods and available supercomputers. Therefore, the extension of AFDMC algorithm to deal with nuclear matter is a significant step forward. Some technical improvements on the calculations presented here, such as the addition to our AV6' of spin–orbit terms and three–body interactions are already underway. The treatment of asymmetric nuclear matter, particularly important for the determination of the properties of neutron stars, is also straightforward, and will be the subject of future exploration.

We acknowledge helpful conversations with M.H. Kalos, P. Faccioli, W. Leidemann, E. Lipparini, and G. Orlandini. This work was in part supported by NSF grant PHY-0456609. Calculations were performed on the HPC facility "BEN" at ECT* in Trento under a grant for Supercomputing Projects.

[1] J. Piekarewicz, Phys. Rev. C **69**, 041301 (2004).
[2] J. Morales, Jr., V. R. Pandharipande, and D. G. Ravenhall, Phys. Rev. C **66**, 054308 (2002).
[3] A. Akmal, V. R. Pandharipande, and D. G. Ravenhall, Phys. Rev. C **58**, 1804 (1998).
[4] J. M. Lattimer and M. Prakash, Science **304**, 536 (2004).
[5] C. Miller, Nature **420**, 31 (2002).
[6] V. R. Pandharipande and R. B. Wiringa, Rev. Mod. Phys. **51**, 821 (1979).
[7] H. Kamada, A. Nogga, W. Glockle, E. Hiyama, M. Kamimura, K. Varga, Y. Suzuki, M. Viviani, A. Kievsky, S. Rosati, et al., Phys. Rev. C **64**, 044001 (2001).
[8] D. Gazit, S. Bacca, N. Barnea, W. Leidemann, and G. Orlandini, Phys. Rev. Lett. **96**, 112301 (2006).
[9] J. Carlson and R. Schiavilla, Rev. Mod. Phys. **70**, 743 (1998).
[10] P. Navrátil, J. P. Vary, and B. R. Barrett, Phys. Rev. Lett. **84**, 5728 (2000).
[11] S. C. Pieper, Nucl. Phys. A **751**, 516 (2005).
[12] S. C. Pieper, K. Varga, and R. B. Wiringa, Phys. Rev. C **66**, 044310 (2002).
[13] J. Carlson, J. Morales, Jr., V. R. Pandharipande, and D. G. Ravenhall, Phys. Rev. C **68**, 025802 (2003).
[14] K. E. Schmidt and S. Fantoni, Phys. Lett. B **446**, 99 (1999).
[15] S. Fantoni, A. Sarsa, and K. E. Schmidt, Phys. Rev. Lett. **87**, 181101 (2001).
[16] A. Sarsa, S. Fantoni, K. E. Schmidt, and F. Pederiva, Phys. Rev. C **68**, 024308 (2003).
[17] S. Gandolfi, F. Pederiva, S. Fantoni, and K. E. Schmidt, Phys. Rev. C **73**, 044304 (2006).
[18] F. Pederiva, A. Sarsa, K. E. Schmidt, and S. Fantoni, Nucl. Phys. A **742**, 255 (2004).
[19] I. Bombaci, A. Fabrocini, A. Polls, and I. Vidaña, Phys. Lett. B **609**, 232 (2005).
[20] S. Zhang and H. Krakauer, Phys. Rev. Lett. **90**, 136401 (2003).
[21] R. B. Wiringa and S. C. Pieper, Phys. Rev. Lett. **89**, 182501 (2002).
[22] R. B. Wiringa, V. G. J. Stoks, and R. Schiavilla, Phys. Rev. C **51**, 38 (1995).
[23] S. Moroni, S. Fantoni, and G. Senatore, Phys. Rev. B **52**, 13547 (1995).
[24] E. Manousakis, S. Fantoni, V. R. Pandharipande, and Q. N. Usmani, Phys. Rev. B **28**, 3770 (1983).
[25] M. Viviani, E. Buendia, S. Fantoni, and S. Rosati, Phys. Rev. B **38**, 4523 (1988).
[26] H. Q. Song, M. Baldo, G. Giansiracusa, and U. Lombardo, Phys. Rev. Lett. **81**, 1584 (1998).
[27] M. Baldo, A. Fiasconaro, H. Q. Song, G. Giansiracusa, and U. Lombardo, Phys. Rev. C **65**, 017303 (2001).